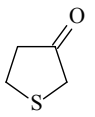
540 **C_4H_6OS** **Thiolan-3-one** **C_1**

MW, *ab initio* calculations

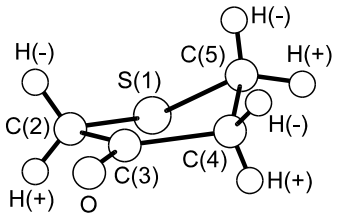
Tetrahydrothiophen-3-one
Dihydro-3(2*H*)-thiophenone



r_0	Å
S(1)–C(2)	1.799(5)
C(2)–C(3)	1.566(17)
C(3)–C(4)	1.487(15)
C(4)–C(5)	1.526(5)
C(2)–H	1.096 [a])
C(3)=O	1.183(7)
C(4)–H	1.097 [a])
C(5)–H	1.095 [a])

θ_0	deg
S(1)–C(2)–C(3)	106.0(7)
S(1)–C(2)–H(+)	111.1 [a])
S(1)–C(2)–H(–)	112.0 [a])
C(2)–C(3)–C(4)	112.2(9)
C(2)–C(3)=O	119.0(16)
C(3)–C(4)–C(5)	108.7(4)
C(3)–C(4)–H(+)	107.1 [a])
C(3)–C(4)–H(–)	109.8 [a])
C(4)–C(5)–S(1)	105.4(2)
C(4)–C(5)–H(+)	113.0 [a])
C(4)–C(5)–H(–)	111.2 [a])
S(1)–C(2)–C(3)=O [b])	–172.0(50)
S(1)–C(2)–C(3)–C(4) [b])	14.0(50)
C(2)–C(3)–C(4)–C(5) [b])	14.0(50)
C(3)–C(4)–C(5)–S(1) [b])	–35.5(50)
C(4)–C(5)–S(1)–C(2) [b])	38.4(20)
C(5)–S(1)–C(2)–C(3) [b])	–29.9(50)
C(2)–C(3)–C(4)–H(+) [b])	–104.1(50)
C(2)–C(3)–C(4)–H(–) [b])	138.5(50)
C(3)–C(4)–C(5)–H(+) [b])	–157.3(50)
C(3)–C(4)–C(5)–H(–) [b])	80.4(50)
C(5)–S(1)–C(2)–H(+) [b])	–146.7(20)
C(5)–S(1)–C(2)–H(–) [b])	92.2(20)

Atom	a_0 [Å]	b_0 [Å]	c_0 [Å]
S(1)	–1.500	–0.438	–0.147
C(2)	0.102	–1.165	0.228
C(3)	1.160	–0.044	–0.049
C(4)	0.533	1.297	–0.191
C(5)	–0.903	1.223	0.321
O	2.351	–0.318	–0.013



Analyses of the moments of inertia describe an envelope ring conformation with C(5) puckered out of the plane established by the remaining heavy atoms.

[a]) Assumed at the values from *ab initio* calculations.
[b]) Dihedral angle.

Torok, C.R., Lavrich, R.J., Tubergen, M.J.: J. Mol. Struct. **612** (2002) 223.